Conduction band offset for $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaN_yAs_{1-y}/GaAs$ systems with the ground state transition at 1.5–1.65 μm

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Conduction band offset for $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaN_yAs_{1-y}/GaAs$ systems with different N contents ($x=2.2\%-3.0\%$ and $y=3.1\%-4.3\%$ of N) has been investigated by contactless electroreflectance spectroscopy supported by theoretical calculations performed within the effective mass approximation. It has been found that $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaN_yAs_{1-y}$ quantum wells (QWs) are promising for laser applications from the point of view of carrier confinement since the conduction band offset (Q_C) for these QWs is between 70% and 75%. In addition, it has been shown that GaNAs/GaAs interface is type I with Q_C between 80% and 90%. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2716366]

The dilute nitrides have garnered great interest as material which can be used in GaAs-based laser diodes operating in the 1.3–1.55 μm optical fiber windows.[1] Recently, a successful realization of 1.5 μm lasers has been achieved by using a GaInNAsSb/GaNAs quantum well (QW) as the active region.[2–4] Currently, there is huge need to improve parameters of these lasers, such as the threshold current density and characteristic temperature T_0 for the threshold current. Therefore, the band gap discontinuity in this system, especially in the valence band, is a crucial issue. The band gap lineup for $Ga_{0.61}In_{0.39}N_{0.017}As_{0.963}Sb_{0.02}/GaN_{0.027}As_{0.973}/GaAs$ QWs has been recognized by photoreflectance spectroscopy in our previous papers[5,6] and it has been concluded that this system has favorable band gap discontinuities for laser applications. Recently, the laser emission of this system has been pushed to longer wavelength increasing the nitrogen concentration in both GaNAs barriers and GaInNAsSb quantum well.[4] However, it was observed that the T_0 for these lasers is low (~70 K). It could imply that this system can have a weak electron (or hole) confinement. In this letter, our works on the band gap discontinuity in GaInNAsSb/GaNAs/GaAs QW system[5,6] have been extended for the recent structures with higher N concentration (4.3% and 3.0% in GaNAs and GaInNAsSb, respectively) in order to explore the origin of the temperature sensitivity in this system.

The $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaN_yAs_{1-y}/GaAs$ QW structures were grown by solid-source molecular beam epitaxy on *n*-type (001) GaAs substrates. The sample is composed of 250-nm-thick GaAs buffer layer, ~50-nm-thick GaAs:N layer with the N concentration of ~0.1%, 21-nm-thick GaNAs steplike barriers (SLBs), 7.5-nm-thick GaInNAsSb QW, and 50-nm-thick GaAs cap layer. Samples used to this study were not annealed (further details of the growth conditions can be found in Refs. [2,4]). The composition of QW layers and the width of the QWs were concluded on the basis of the secondary ion mass spectroscopy and the high resolution x-ray diffraction measurements. Three samples, labeled as S1, S2, and S3, with different N contents in QW and SLBs are presented in this letter. The content for sample S1, S2, and S3 is 2.2%, 2.8%, and 3.0% of N in GaInNAsSb QW and 3.1%, 3.8%, and 4.3% of N in GaNAs SLBs, respectively. A conventional experimental setup was applied for obtaining contactless electroreflectance (CER) spectra.[7–9]

In Fig. 1 the part of the CER spectrum below the GaAs:N-related transition is connected with GaInNAsSb/GaNAs QW. In this spectral region two portions of optical transitions are visible. The first portion is

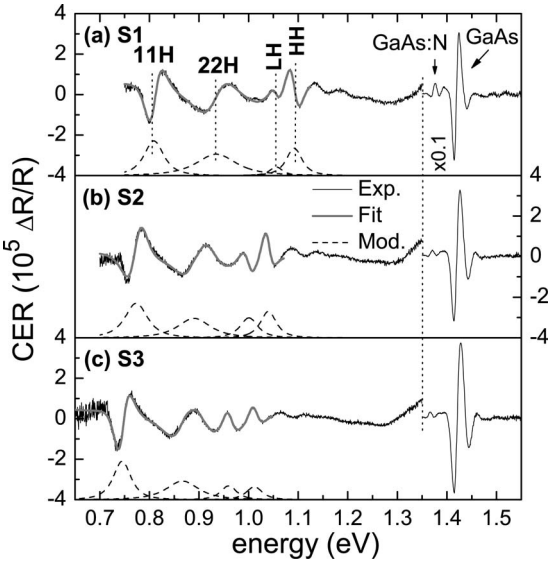

FIG. 1. Room temperature CER spectra (thin solid lines) of (a) S1, (b) S2, and (c) S3 structures together with fitting curves (thick solid lines) and the modulus of the individual lines (dashed lines).

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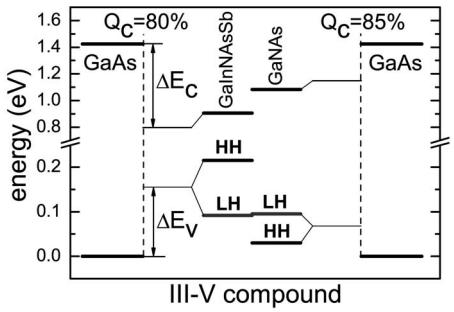

FIG. 2. Band lineup for GaAs–$Ga_{0.62}In_{0.38}N_{0.028}As_{0.963}Sb_{0.009}$–$GaN_{0.038}As_{0.962}$–GaAs system. The conduction band offset Q_C is defined for unstrained materials as marked in this figure (see also Refs. 5–7).

associated with optical transitions between energy levels confined in GaInNAsSb/GaNAs QW (transitions labeled as 11H and 22H:*nm*H denotes the transition between *n*th heavy-hole valence subband and *m*th conduction subband) and the second is associated with optical transitions between energy levels confined above GaNAs SLBs (transitions labeled as LH and HH). The nominally forbidden transitions (e.g., 12H or 21H) can be neglected in this case since the lack of strong built-in electric fields is expected for these structures in the GaInNAsSb QW region.

In order to extract energies of the optical transitions, standard fitting procedure has been applied and modulus of CER resonances has been plotted in Fig. 1, similar in our previous papers.[7–9] The identification of the resonances was possible on the basis of the calculations performed in the framework of the effective mass approximation with material parameters taken from Refs. 10 and 11 except the electron effective mass which was assumed to be $0.09m_0$ and $0.11m_0$ for GaInNAsSb and GaNAs, respectively. Such an assumption indicates ~50% increase in the electron effective mass in comparison to N-free compounds and is in accordance with the band anticrossing (BAC) model,[12] our previous analysis,[7–9] and experimental data[13,14] obtained for similar compounds. The electron effective mass was not varied with the increase in the N concentration since small changes in the electron effective mass are expected in this regime of nitrogen contents (see BAC model and Ref. 15). The band gap energy for the GaNAs barriers was extracted directly from the energy position of LH and HH transitions taking into account strains, as shown in Fig. 2. The Q_C is the "so-called" chemical band offset and is defined by

$$Q_C = \frac{\Delta E_C}{\Delta E_C + \Delta E_V} 100\%, \tag{1}$$

where ΔE_C and ΔE_V are the discontinuities for conduction and valence bands of unstrained materials (see Fig. 2). Other relevant details of the calculations can be found in Refs. 7–9.

Figure 3 shows a comparison between experimental data and theoretical calculations performed for various Q_C for the GaInNAsSb/GaNAs interface. The energy difference between the 22H and 11H transitions is analyzed in this figure since it is one of the best criteria for matching experimental data with theoretical calculations. The best agreement for the three QWs is obtained with $70\% < Q_C < 75\%$. This value is determined directly for the GaInNAsSb/GaNAs interface. Usually, semiconductor structures are grown on binary substrates. Therefore more universal/appropriate approach is to investigate the Q_C between the alloy and a binary compound.

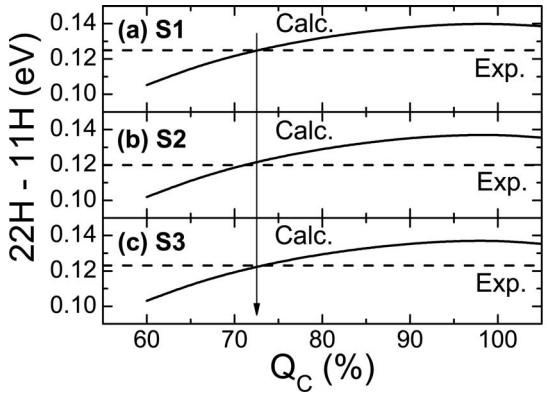

FIG. 3. Comparison of theoretical calculations (solid curves) with experimental data (horizontal dashed lines) for (a) S1, (b) S2, and (c) S3 structures.

The Q_C for GaInNAsSb/GaAs and GaNAs/GaAs interfaces has been investigated in few papers[8,9,16,17] and hence some predictions concerning the Q_C for the GaInNAsSb/GaNAs interface can be done. In order to compare the results obtained in this letter with literature data the following equation has been extracted from Eq. (1) written for the three interfaces in the GaInNAsSb/GaNAs/GaAs system:

$$Q_C^{BC} = \frac{Q_C^{AC}(E_g^A - E_g^C) - Q_C^{AB}(E_g^A - E_g^B)}{E_g^A - E_g^C - E_g^A + E_g^B}. \tag{2}$$

The notation A, B, and C in Eq. (2) corresponds to GaAs, GaNAs, and GaInNAsSb, respectively. Assuming that the Q_C for the GaInNAsSb/GaNAs interface is higher than 70% and smaller than 75% (see Fig. 3), the Q_C for the GaInNAsSb/GaAs interface can be expressed by the Q_C related to the GaNAs/GaAs interface, as shown in Fig. 3. Next taking into account literature data for the GaInNAsSb/GaAs system some conclusions concerning the Q_C for GaNAs/GaAs system can be obtained and vice versa.

In the case of GaInNAsSb/GaAs QWs of similar contents, it has been reported that the Q_C is ~80%.[9,17] Moreover, it is well known that Sb-free QWs with similar In and N contents also have the Q_C~80%.[18,19] So the Q_C for the $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}$/GaAs interface is rather well specified and is plotted in Fig. 4 by horizontal dashed line. In the case of GaNAs/GaAs interface, no band gap discontinuity for the valence band ($Q_C = 100\%$) is expected for unstrained materials within the BAC model. However, recent studies have shown that GaNAs/GaAs QWs with $1.2\% < N < 2.4\%$ are structures of type I for both electrons and holes and the Q_C for this system is between 80% and 90%.[8] In this letter we can conclude how is the Q_C for GaNAs/GaAs interface with high N content (3.1%–4.3%). According to Fig. 4 it has been found that this interface is type I with the Q_C between 80% and 90%. Note that the GaInNAsSb/GaNAs/GaAs system is very sensitive to the band gap discontinuity at the GaNAs/GaAs interface. Assuming $Q_C = 100\%$ for the GaNAs/GaAs interface, the electron potential for GaInNAsSb/GaNAs QW is shallow and confines only one state whereas the 22H transition is clearly observed in CER spectra.

For QW laser design, the relevant parameters are the band gap discontinuities in the strained system, namely, the values of ΔE_C^* and ΔE_V^{HH} (see Refs. 7–9), for the conduction and heavy-hole QWs, respectively (see Fig. 5). Note that

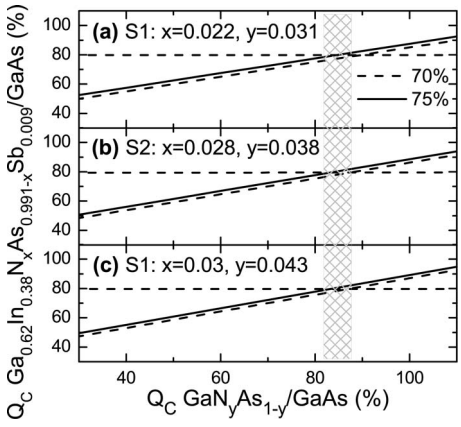

FIG. 4. Relations between the Q_C for the $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaN_yAs_{1-y}$ interface and $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaAs$ and $GaN_yAs_{1-y}/GaAs$ interfaces. It is assumed after Refs. 9 and 17 that Q_C for the $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaAs$ interface is 80% with 5% accuracy (see horizontal dashed lines). In general, the conduction band offset at the $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaAs$ interface can vary for the three samples since the N concentration in the $Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}$ quantum well increases from $x=0.022$ to $x=0.03$. However, the expected changes should be much smaller than 5%. The conduction band offset for GaNAs/GaAs interfaces is treated as an unknown parameter in this case.

when the N content for GaInNAsSb quantum well is increased the band gap discontinuities also increased due to the band gap and strain reduction in this layer (it is strong band gap tuning). But when the N content for GaNAs barriers is increased, the band gap discontinuities decreased because of the band gap reduction. However in this case, the increased tensile strain weakens the band gap reduction for GaNAs barriers. Finally, the band gap discontinuities for samples S1, S2, and S3 are bigger that the previous ones which were obtained for samples with smaller N concentration.[5,6] The determined band gap discontinuities are very promising from the viewpoint of T_0 parameter and they do not explain such low value for this parameter. We believe that the strong temperature sensitivity of this system is associated with other phenomena such as nonradiative recombination via defect states in GaNAs barriers and/or Auger processes. Thus, future work may focus on the improvement of the optical quality of GaNAs and GaInNAsSb layers since the band gap discontinuity at GaInNAsSb/GaNAs interface ensures good confinement for both electrons and holes.

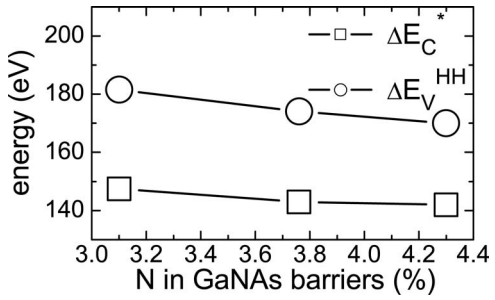

FIG. 5. Band gap discontinuities for samples S1, S2, and S3 structures $[Ga_{0.62}In_{0.38}N_xAs_{0.991-x}Sb_{0.009}/GaN_yAs_{1-y}/GaAs$ systems with different N contents ($x=0.022-0.03$ and $y=0.031-0.043$) as a function of N concentration in GaNAs barriers].

In conclusion, it has been found that the Q_C for the investigated GaInNAsSb/GaNAs QWs is between 70% and 75%. This value is consistent with the $Q_C=80\%$ and $Q_C=80\%-90\%$ for GaInNAsSb/GaAs and GaNAs/GaAs interfaces, respectively. It means that from the viewpoint of T_0 parameter, the GaInNAsSb/GaNAs system has the ability to effectively confine both electrons and holes.

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